Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (II)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
Rh(1)	0	0.13238 (3)	1/4	0.04222 (12)
N(1)	−0.08157 (12)	−0.0477 (3)	0.2250 (2)	0.0477 (5)
N(2)	−0.14580 (13)	−0.2118 (3)	0.12792 (15)	0.0490 (6)
C(1)	−0.1343 (2)	−0.0959 (5)	0.2825 (2)	0.0653 (9)
C(21)†	−0.2066 (4)	−0.1394 (17)	0.2445 (5)	0.066 (2)
C(22)‡	−0.1882 (12)	−0.2208 (39)	0.2586 (11)	0.065 (5)
C(3)	−0.2060 (2)	−0.2520 (5)	0.1756 (2)	0.0761 (12)
C(4)	−0.1481 (2)	−0.2445 (5)	0.0414 (2)	0.0623 (8)
C(5)	−0.0744 (2)	−0.1894 (6)	0.0190 (2)	0.0780 (11)
C(6)	−0.0473 (2)	−0.0721 (5)	0.0834 (2)	0.0633 (9)
C(7)	−0.09274 (15)	−0.1087 (3)	0.1536 (2)	0.0448 (6)
C(8)	0.0417 (3)	0.4474 (5)	0.1726 (3)	0.099 (2)
C(9)	0.0783 (2)	0.3128 (5)	0.2255 (3)	0.0710 (10)
C(10)	0.0746 (2)	0.3018 (4)	0.3070 (3)	0.0709 (10)
C(11)	0.0355 (3)	0.4152 (6)	0.3574 (3)	0.0931 (14)
P(1)	1/4	1/4	1/2	0.0619 (3)
F(1)	0.3331 (2)	0.2424 (6)	0.4860 (2)	0.1489 (15)
F(2)	0.2606 (2)	0.1064 (3)	0.5619 (2)	0.1218 (12)
F(3)	0.2330 (2)	0.1307 (3)	0.4275 (2)	0.1227 (13)

† Site occupancy 0.73 (3).
‡ Site occupancy 0.27 (3).

Table 4. *Selected geometric parameters* (Å, °) *for* (II)

X represents the midpoint of the C(9)═C(10) double bond.

Rh(1)—C(10)	2.124 (3)	Rh(1)—X	2.019 (3)
Rh(1)—N(1)	2.129 (2)	C(9)—C(10)	1.359 (6)
Rh(1)—C(9)	2.136 (3)		
N(1)—Rh(1)—N(1^{i})	90.4 (1)	X^{i}—Rh(1)—X	87.6 (2)
N(1)—Rh(1)—X	91.1 (2)		

Symmetry code: (i) $-x, y, \frac{1}{2} - z$.

Program used to solve structures: *SHELXS*86 (Sheldrick, 1990). Program used to refine structures: *SHELXL*93 (Sheldrick, 1994).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HR1015). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis(dimethylglyoximato-*N*,*N*′)(triphenylphosphine-*P*)vinylrhodium(III)

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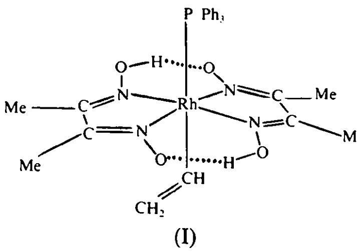
Abstract

The title structure {bis[2,3-butanedial dioximato-(1 −)-*N*,*N*′](triphenylphosphine-*P*)vinylrhodium(III), [$Rh(C_2H_3)(C_4H_7N_2O_2)_2(C_{18}H_{15}P)$]} consists of discrete complexes in which the Rh atom displays distorted octahedral coordination, where the two dimethylglyoxime ligands lie in the equatorial plane and the vinyl and triphenylphosphine groups occupy the axial positions. The Rh atom is displaced by 0.123 (1) Å from the mean plane through the four oxime N donors. The average Rh—N distance is 1.957 (2) Å, while the axial Rh—P and Rh—C distances are 2.447 (1) and 2.035 (3) Å, respectively. Comparison of the results with those obtained previously for the analogous ethyl compound indicates a lower *trans* influence of the vinyl ligand in the axial P—Rh—C fragment.

Comment

This work is part of a more general study aimed at understanding the mutual influence of ligands in organometallic compounds (Steinborn, 1992). The *trans* influence of organic ligands is of particular interest. Recent NMR investigations of complexes [$Rh(dmgH)_2(PPh_3)R$] (dmgH is the monoanion of dimethylglyoxime, R is an organo group) (Steinborn & Ludwig, 1993) demonstrates that the *trans* influence of the organo group R, as measured by $^1J(^{103}Rh–^{31}P)$ coupling constants, is nearly the same for the sp^3-hybridized ethyl group and the sp^2-

hybridized vinyl and phenyl groups. In order to examine whether there is a relationship between the *trans* influence of organo groups measured both spectroscopically by NMR and derived from structural data, the crystal structure of the ethyl complex $[Rh(dmgH)_2(PPh_3)Et]$ was determined and reported (Kettmann, Dunaj-Jurčo, Steinborn & Ludwig, 1994). The crystal structure of the vinyl analogue (I) is reported here. The molecular structure and the numbering scheme is shown in Fig. 1.



(I)

The crystal contains discrete molecules in which the Rh atom exhibits a distorted octahedral stereochemistry, with four oxime N donors in equatorial positions. The two dimethylglyoxime ligands are present as monoanionic species and are stabilized by two intramolecular hydrogen bonds acting between the atoms O(1) and O(4) [O···O = 2.587 (2) Å] and between the atoms O(2) and O(3) [O···O = 2.657 (2) Å]. Based on the H-atom positions (not refined) as determined from a $\Delta\rho$ map, the latter hydrogen bond is typically unsymmetrical [O(3)—H = 0.99, O(2)—H = 1.79 Å] while the former is almost symmetrical [O(4)—H = 1.25, O(1)—H = 1.38 Å].

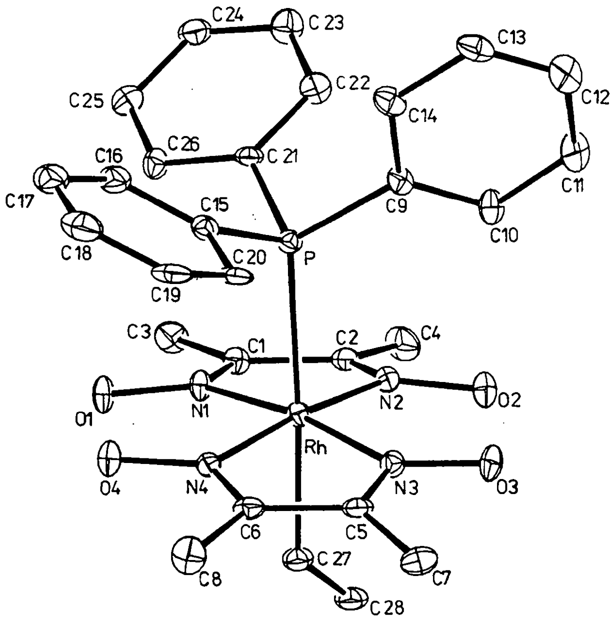


Fig. 1. Perspective drawing of the title compound showing the atom-numbering scheme.

The four Rh—N bond distances are equal within the limits of experimental error, with a mean value of 1.957 (2) Å. This value is shorter than that in the closely related $[RhCl(dmgH)_2(PPh_3)]$ complex [1.992 (4) Å; Cotton & Norman, 1971] but equal to that found in the ethyl analogue [1.955 (6) Å; Kettmann *et al.*, 1994]. The $Rh(dmgH)_2$ system is not strictly planar; the two $dmgH^-$ ligands are tilted away from the triphenylphosphine ligand so that their normal vectors are at an angle of 15.1 (2)° to each other. As a result, though the four oxime N donors are coplanar to within ±0.018 Å, the Rh atom is displaced by 0.123 (1) Å from their mean plane toward the P atom. The $dmgH^-$ ligands themselves are not strictly planar; the lack of planarity originates from a twisting of the two halves of the ligand about the central C—C bond, the twist angles being 7.2 (2) and 6.9 (2)° for ligands N(1), N(2), O(1), O(2), C(1)–C(4) and N(3), N(4), O(3), O(4), C(5)–C(8), respectively.

As mentioned previously, the *trans* influence of the axial ligands, namely the σ-bonded vinyl group and the PPh_3 moiety, is of special interest here. The Rh—P and Rh—C bond lengths are 2.447 (1) and 2.035 (3) Å, respectively, and the P—Rh—C angle is 177.4 (1)°. Similar structural features have also been found for chlorobis(2-nitrophenyl-*C*,*O*)(triphenylphosphine)rhodium(III), another complex in which an sp^2-hybridized C atom (the β-C atom of the 2-nitrophenyl ligand) lies opposite the PPh_3 group (Vicente, Martin, Solans & Font-Altaba, 1989), as well as for the complex $[Rh(dmgH)_2(PPh_3)Et]$ (Kettmann *et al.*, 1994).

The Rh—C bond distance [2.035 (3) Å] is within the range of other known Rh—C(sp^2) bond distances: *cf.* 2.04 (2) Å in chlorobis(2-nitrophenyl-*C*,*O*)(triphenylphosphine)rhodium(III) (Vicente *et al.*, 1989) and 2.00 (1) Å in $[\{(C_5Me_5)Rh(\mu\text{-}CH_2)(CH{=}CH_2)\}_2]$ (Martinez, Gill, Adams, Bailey, Saez, Sunley & Maitlis, 1990).

The Rh—C and the Rh—P bond distances in the vinyl complex $[Rh(dmgH)_2(PPh_3)R]$ ($R = CH{=}CH_2$) are slightly shorter than those in the ethyl complex (R = Et); Rh—C 2.035 (3) *versus* 2.064 (7) Å and Rh—P 2.447 (1) *versus* 2.461 (2) Å. This corresponds with the difference in radii of sp^2- and sp^3-hybridized C atoms and with the *trans* influence of R (vinyl < ethyl) (Appleton, Clark & Manzer, 1973; Steinborn, Taube & Radeglia, 1988), respectively.

The C═C bond distance [C(27)═C(28) 1.271 (4) Å] is even shorter than the C═C bond in ethylene [1.336 (2) Å; Bartell, Roth, Hollowell, Kuchitsu & Young, 1965], but it is within the range of other vinyl complexes: *cf.* 1.24 (5) Å in

$[Pt(PPh_3)_2(MeC{=}CMeH)]OTf$ (Stang, Kowalski, Schiavelli & Longford, 1989), 1.25 (2) Å in $[\{(C_5Me_5)Rh(\mu\text{-}CH_2)(CH{=}CH_2)\}_2]$ (Martinez *et al.*, 1990), and 1.36 (2) and 1.37 (2) Å in *trans*- and *cis*-$[Pt(PPh_3)_2(C{\equiv}C\text{-}^tBu)(CMe{=}CH_2)]$ (Stang & Kowalski, 1989), respectively.

More structural data are needed to evaluate the relationship of the *trans* influence in rhodium complexes $[Rh(dmgH)_2(PPh_3)R]$ derived from NMR and structural data. In this respect, the X-ray structure analysis of the phenylacetylide complex ($R = C{\equiv}CPh$) is in progress.

Experimental

Crystal data

$[Rh(C_2H_3)(C_4H_7N_2O_2)_2\text{-}(C_{18}H_{15}P)]$
$M_r = 622.5$
Monoclinic
$P2_1/c$
$a = 9.703\ (5)$ Å
$b = 11.014\ (4)$ Å
$c = 25.218\ (9)$ Å
$\beta = 97.91\ (4)°$
$V = 2669.4\ (8)$ Å^3
$Z = 4$
$D_x = 1.548$ Mg m^{-3}
$D_m = 1.55\ (1)$ Mg m^{-3}
D_m measured by flotation in $CHBr_3$–cyclohexane

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 15 reflections
$\theta = 7–15°$
$\mu = 0.73$ mm^{-1}
$T = 295$ K
Prism
0.50 × 0.40 × 0.20 mm
Brownish yellow
Crystal source: slow evaporation of an acetone solution at room temperature

Data collection

Syntex $P2_1$ diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical
$T_{min} = 0.83$, $T_{max} = 1.00$
6711 measured reflections
5950 independent reflections
4199 observed reflections [$I \geq 2\sigma(I)$]

$R_{int} = 0.032$
$\theta_{max} = 27.5°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 14$
$l = -32 \rightarrow 32$
2 standard reflections monitored every 100 reflections
intensity variation: ±4%

Refinement

Refinement on F
$R = 0.038$
$wR = 0.044$
$S = 1.17$
4199 reflections
343 parameters
H-atom parameters not refined

$w = 1/[\sigma^2(F_o) + 0.025|F_o|^2]$
$(\Delta/\sigma)_{max} = 0.08$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Rh(1)	0.2096 (1)	0.1403 (1)	0.1639 (1)	2.48 (1)
P(1)	0.1508 (1)	0.3143 (1)	0.1048 (1)	2.48 (1)
O(1)	0.0954 (2)	−0.0217 (2)	0.0803 (1)	3.43 (4)
O(2)	0.4980 (2)	0.2054 (2)	0.1893 (1)	3.76 (5)
O(3)	0.3294 (2)	0.2749 (2)	0.2582 (1)	3.97 (5)
O(4)	−0.0728 (2)	0.0545 (2)	0.1442 (1)	3.48 (5)
N(1)	0.2096 (2)	0.0322 (2)	0.1021 (1)	2.64 (5)
N(2)	0.4056 (2)	0.1470 (2)	0.1544 (1)	2.64 (5)
N(3)	0.2119 (2)	0.2267 (2)	0.2320 (1)	3.00 (6)
N(4)	0.0180 (2)	0.1176 (2)	0.1779 (1)	2.57 (5)
C(1)	0.3289 (3)	0.0159 (2)	0.0855 (1)	2.93 (6)
C(2)	0.4426 (2)	0.0803 (2)	0.1165 (1)	3.08 (6)
C(3)	0.3445 (3)	−0.0639 (3)	0.0397 (1)	4.27 (8)
C(4)	0.5903 (3)	0.0654 (3)	0.1091 (1)	5.11 (10)
C(5)	0.1007 (3)	0.2213 (2)	0.2545 (1)	3.40 (7)
C(6)	−0.0144 (2)	0.1582 (2)	0.2226 (1)	3.25 (6)
C(7)	0.0910 (4)	0.2634 (3)	0.3097 (1)	5.37 (10)
C(8)	−0.1512 (3)	0.1388 (3)	0.2401 (1)	5.32 (10)
C(9)	0.2210 (3)	0.4625 (2)	0.1229 (1)	2.99 (6)
C(10)	0.3500 (3)	0.4728 (2)	0.1534 (1)	3.73 (7)
C(11)	0.4109 (3)	0.5852 (3)	0.1621 (1)	4.72 (8)
C(12)	0.3420 (4)	0.6869 (3)	0.1426 (1)	4.79 (9)
C(13)	0.2164 (3)	0.6788 (2)	0.1134 (1)	4.60 (9)
C(14)	0.1520 (3)	0.5653 (2)	0.1025 (1)	3.91 (8)
C(15)	−0.0344 (2)	0.3434 (2)	0.0951 (1)	3.07 (6)
C(16)	−0.1217 (3)	0.3264 (3)	0.0488 (1)	4.66 (9)
C(17)	−0.2624 (3)	0.3436 (3)	0.0463 (2)	5.77 (11)
C(18)	−0.3149 (3)	0.3826 (3)	0.0904 (2)	5.99 (12)
C(19)	−0.2281 (3)	0.4028 (3)	0.1379 (1)	5.11 (9)
C(20)	−0.0897 (3)	0.3825 (3)	0.1400 (1)	4.18 (8)
C(21)	0.2030 (2)	0.2936 (2)	0.0390 (1)	2.81 (6)
C(22)	0.1464 (3)	0.2017 (2)	0.0051 (1)	3.28 (7)
C(23)	0.1925 (3)	0.1841 (3)	−0.0434 (1)	4.26 (9)
C(24)	0.2991 (3)	0.2532 (1)	−0.0577 (1)	4.30 (8)
C(25)	0.3577 (3)	0.3418 (3)	−0.0240 (1)	4.51 (8)
C(26)	0.3083 (3)	0.3621 (3)	0.0236 (1)	3.81 (7)
C(27)	0.2538 (3)	−0.0094 (2)	0.2105 (1)	3.46 (7)
C(28)	0.3706 (3)	−0.0565 (3)	0.2283 (1)	4.09 (8)

Table 2. *Selected geometric parameters* (Å, °)

Rh(1)—P(1)	2.447 (1)	N(1)—O(1)	1.310 (3)
Rh(1)—C(27)	2.035 (3)	N(2)—O(2)	1.333 (3)
Rh(1)—N(1)	1.960 (2)	N(3)—O(3)	1.345 (3)
Rh(1)—N(2)	1.951 (2)	N(4)—O(4)	1.333 (3)
Rh(1)—N(3)	1.962 (2)	N(1)—C(1)	1.297 (3)
Rh(1)—N(4)	1.956 (2)	N(2)—C(2)	1.294 (3)
P(1)—C(9)	1.804 (2)	N(3)—C(5)	1.287 (3)
P(1)—C(15)	1.808 (3)	N(4)—C(6)	1.290 (3)
P(1)—C(21)	1.814 (2)	C(1)—C(2)	1.447 (3)
C(27)—C(28)	1.271 (4)	C(5)—C(6)	1.460 (4)
N(1)—Rh(1)—N(2)	79.6 (1)	Rh(1)—C(27)—C(28)	129.9 (2)
N(3)—Rh(1)—N(4)	78.5 (1)	Rh(1)—P(1)—C(9)	120.5 (1)
P(1)—Rh(1)—N(1)	91.0 (1)	Rh(1)—P(1)—C(15)	111.4 (1)
P(1)—Rh(1)—N(2)	92.6 (1)	Rh(1)—P(1)—C(21)	112.8 (1)
P(1)—Rh(1)—N(3)	97.3 (1)	C(9)—P(1)—C(15)	101.9 (1)
P(1)—Rh(1)—N(4)	93.6 (1)	C(9)—P(1)—C(21)	101.9 (7)
P(1)—Rh(1)—C(27)	177.4 (1)	C(15)—P(1)—C(21)	107.2 (1)

All calculations were performed with the *NRC Crystallographic Programs for the IBM360 System* (1973). All H atoms were located from difference Fourier maps and included as fixed contributors to the F_c calculation with B_{iso} set to 0.5 Å^2 higher than the B_{eq} value of the corresponding C atoms.

Financial support from the Deutsche Forschungsgemeinschaft and the Fonds der Chemischen Industrie is gratefully acknowledged.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, interatomic bond distances and least-squares-planes data have been deposited with the IUCr (Reference: KA1060). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1994). C50, 1430–1432

{[(1*R*,2*S*,3*R*,6*R*)-2-(*tert*-Butyldimethylsilyloxymethyl)-6-(2-furyl)-3-methyl-4-oxocyclohexyl](methoxy)methylene}pentacarbonyltungsten(0)

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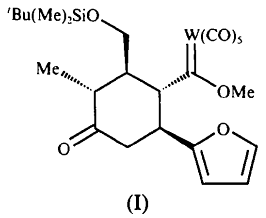
Abstract

The structure and absolute configuration of the title compound, $[W(CO)_5(C_{20}H_{32}O_4Si)]$, is reported. The W atom has distorted octahedral coordination defined by one carbene and five carbonyl ligands.

Comment

Fischer-carbene complexes (Fischer & Maasbol, 1964) are well known for their ability to produce a wide range of reactions (Wulff *et al.*, 1990) which are used increasingly in organic synthesis. For example, they promote benzannulation reactions between α,β-unsaturated complexes and alkenes, cyclopropanation of olefins, cycloaddition of unsaturated complexes to 1,3-dienes, and photolytic reactions. In an earlier paper we reported (Barluenga *et al.*, 1994) a highly stereoselective [4+2] cycloaddition reaction between chiral 2-amino-1,3-dienes and α,β-unsaturated Fischer-carbene complexes of tungsten. Since the elucidation of the absolute configuration of these complexes is essential in order to understand the detailed mechanism of selective formation of one of the possible enantiomers, a single-crystal X-ray diffraction study of the title complex (I) has been carried out.



(I)

The complex contains a central W atom bonded to one carbene and five carbonyl groups. The W atom is thus coordinated by six C atoms with a W—C(carbene) bond length of 2.171 (3) Å and a mean W—C(CO) bond length of 2.037 (2) Å. The stereochemistry around the W atom is only approximately octahedral. The maximum distortions from ideal octahedral geometry are shown by the angles C23—W1—C25 and C1—W1—C22 of 85.1 (2) and 98.3 (2)°, respectively.

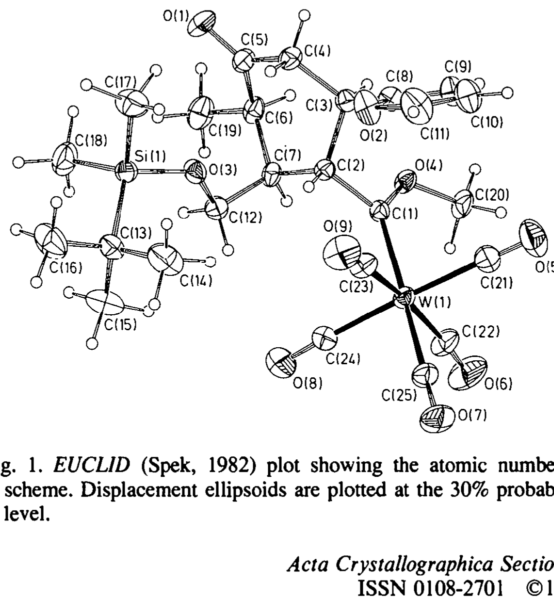


Fig. 1. *EUCLID* (Spek, 1982) plot showing the atomic numbering scheme. Displacement ellipsoids are plotted at the 30% probability level.

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